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NUMERICAL SIMULATION OF THE ALPHA CASE AS A QUALITY CRITERION  
FOR THE INVESTMENT CASTING OF SMALL, THIN-WALLED TITANIUM PARTS

#### SUMMARY

As yet, no casting and solidification process put forward for the investment casting of titanium allows castings to be produced without a hardness increase in the surface zone. Casting quality depends to a not insignificant extent on the structure of this surface zone. For these reasons, the alpha case was selected as a quality criterion.

On the basis of the diffusion kinetics of the alpha case components, a criterion function using simulation and modelling techniques to predict the alpha case quality criterion was developed. Calculations were compared with experimental results for the titanium casting and solidification process developed at the Institute, and iteratively optimized.

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## 1 - THE ALPHA CASE - WHAT IS IT - HOW AND WHY DOES IT FORM?

The selection of the mould material is an important consideration when casting reactive metals (1,2,3,4,6). Reduction of most refractory oxides by molten titanium produces reaction zones rich in oxygen, and known as the alpha case (fig. 1) (4,5,6). In addition to combining with titanium to form oxides in the film or scale, oxygen may also dissolve in the titanium interstitially, to the extent of more than 10% wt. Interstitially-dissolved oxygen tends to stabilize the alpha (hcp) phase of titanium. One of the prominent features of oxygen-contaminated material is therefore an alpha-stabilized surface zone immediately below the oxide scale (7,8,9).

The resulting "case" formed at the mould-metal interface is a material discontinuity, which normally has to be removed owing to its characteristically high-hardness inner scale. X-ray diffraction studies reveal an expanded c/a ratio in the inner scale.

The thickness of the layer increases with the time during which a high temperature is maintained in the mould-metal interface, limiting application of high mould pre-heat temperatures to thin sections. The depth of contamination is dependent on the section, with thick walls favouring greater penetration.

Surface contamination of this type may result in reduced tensile strength, flexural strength and fatigue strength, and severely affect susceptibility to stress-corrosion cracking (5,7).

Removal of the case poses problems on complex castings with varying section size.

Wax pattern tooling also has to be engineered for both the conventional casting allowance of the alloy and an extra acid

metal removal allowance to permit removal of the metal-mould reaction layer. All wax patterns and as-cast parts are therefore slightly oversize, final tolerances being achieved only in the acid cleaning operation (6,7).

## 2 - CORRELATION BETWEEN ALPHA CASE AND CASTING PROPERTIES

Tensile strength is slightly higher and strain considerably higher in non-alpha-case as opposed to alpha-case specimens of the same material. As well as reducing ductility, the alpha case may be a contributing factor in stress crack propagation. Alpha-case castings possess only extremely low fatigue limits as compared to chemically milled castings. Hot isostatic pressing after chemical milling further enhances this advantage. The bending test also reveals a substantially lower bending angle for material with a brittle surface zone.

The high hardness of the surface zone could, however, result in certain advantages for components subjected to wear. A further not inconsiderable disadvantage as opposed, for example, to steel investment casting, lies in the generally inferior accuracy to size of investment-cast titanium, owing to differential alpha case formation and the resulting differential removal rates when the alpha case is eliminated.

## 3 - EXPERIMENTAL PROCEDURE

### 3.1 - Overview

In view of the above observations, the alpha case can be used as a measure of casting quality, insofar as appropriate quality

values are defined for given depths of hardness penetration. A simple example, simultaneously acting as a "checking-device" is a casting wedge (Fig. 2). The influence of the mould material, casting and mould pre-heat temperatures and, especially in the case of the casting wedge, the geometrical influence on the extent of surface zone hardening are all relatively easy to determine. Alpha-case wedges integrally cast with the part can show whether post-processing by means of chemical milling has succeeded in removing the case completely.

### 3.2 - Casting the Alpha-case wedge

Fabrication of the investment mould is by the lost wax process, with application of the ceramic front layer to the wax model cluster using the investment casting shell mould technique (Fig. 3). The compacting method is used to introduce the backfill as a supporting material, for example in the case of conventional packaging for jewellery casting. De-waxing and firing are carried out in conventional furnaces.

Casting of the moulds takes place in a vacuum high-frequency induction spinning machine designed for relatively small melt masses, max 400 g (Fig. 4).

### 3.3 - Correlation between Alpha-case formation and process parameters

The influence of process parameters on the formation of the alpha case for centrifugal investment casting of titanium of small, thin-walled parts was investigated at the Foundry Institute.

After casting, the casting wedge was removed in such a way that the extent of surface zone hardening could be determined in relation to wall thickness (Fig. 5).

A comparison between the hardness distribution (measuring points with fitted curve) and the micrograph (vertical broken line) shows that the extent of alpha-case formation can be determined by either method. The left-hand diagram in Fig. 5 shows the thickness of the layer in a thinner-walled section of the wedge, the right-hand diagram the equivalent value for the thickest-walled section. There is less alpha-case formation in thinner sections.

The influence of the process parameters on formation of the alpha case is indicated below. The following significant influencing variables were investigated:

- 1 Mould pre-heat temperature;
- 2 Casting temperature;
- 3 Position of the casting in the mould;
- 4 Moment of acceleration in the centrifugal casting process.

Fig. 6 indicates the influence of mould pre-heat temperature and casting temperature on formation of the layer. Increased temperatures lead to greater surface brittleness.

The effects of the casting position in the mould and the filling rate of the mould cavity, shown here as functions of the moment of acceleration of the spinning machine arm, are demonstrated in Fig. 7. It will be evident that melt admission conditions during filling also play a role.

#### 4 - NUMERICAL SIMULATION AS A TOOL FOR CASTING OPTIMIZATION

As well as meeting extreme strength requirements, highly-stressed titanium investment castings must increasingly conform to the highest accuracy-to-size-specifications, comparable for example with those for investment-cast steel parts. These two demands can be met only if the exact extent of the unavoidable alpha-case layer of titanium castings is known, and the layer can be removed with corresponding precision.

Prediction of alpha-case thickness is therefore helpful, and computer simulation offers a possible method.

Using a FEM programme, both the process parameters and the alpha-case thickness can be predicted.

The component geometry and the thermophysical and thermodynamic data (Diagram 1) of the casting metal and mould material are entered in the computer programme. The part is then meshed on the finite element principle (Fig. 8) and the thermophysical data calculated in accordance with the temperature distribution or cooling curves (Fig. 9).

Using criterion functions, the hardened layer can then be calculated from the temperature curves (Fig. 10). The criterion functions take account of the various influences of the process parameters and part geometry on the formation of the layer.

As already noted, the programme simultaneously enables, for example, temperature curves in the casting to be visualized. By modifying the simulated process parameters and ingate and feeder system, the user can perform a "cold cast". Time consuming and cost-intensive test series are shortened or eliminated.

5 - REFERENCES

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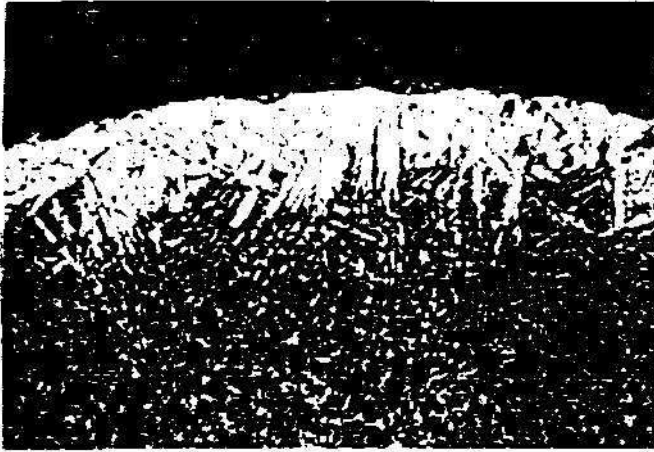


Fig. 1 - Commercially pure titanium with 0.3% Oxygen. The light margin represents the so-called alpha case

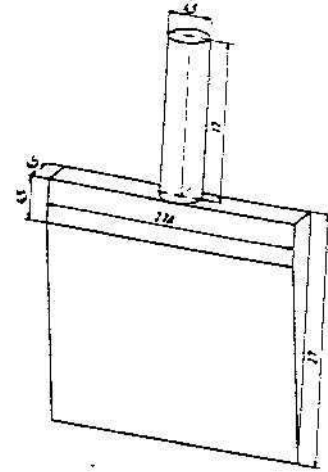


Fig. 2 - Casting wedge used to investigate the relationship between the extent of alpha

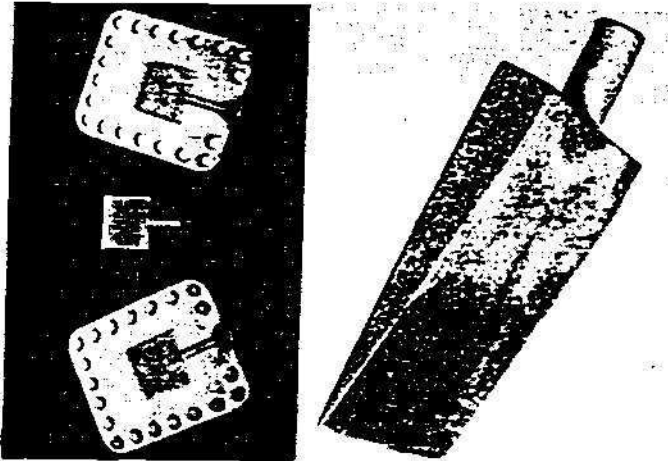


Fig. 3 - Investment casting method: injection mould, wax pattern, cast specimen

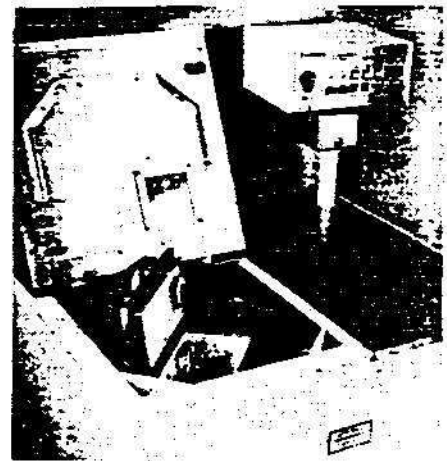


Fig. 4 - High frequency induction centrifuge caster (by courtesy of Linn Elektronik, Federal Republic of Germany)

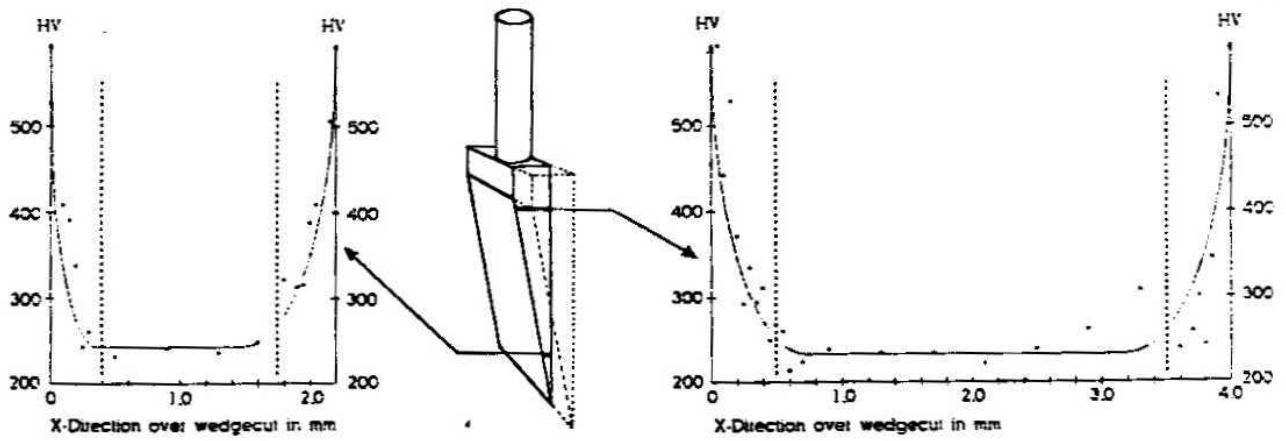


Fig. 5 - Alpha-case development and location in casting wedge. Right: deeper penetration due to thicker section; left: opposite effect

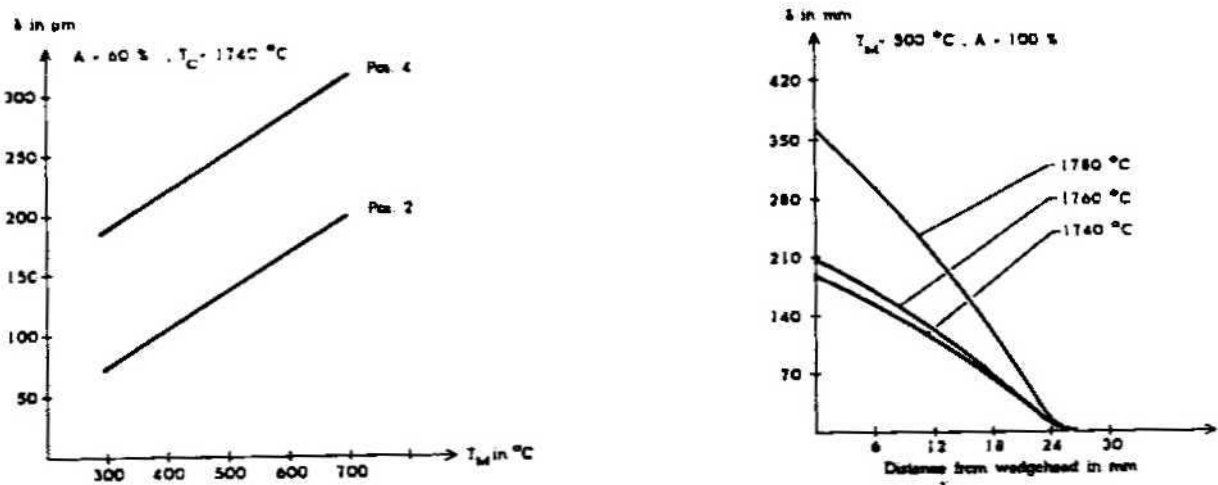


Fig. 6 - Alpha-case as a function of mould Pre-heating temperature (left) and casting temperature (right) at a defined point in the casting wedge

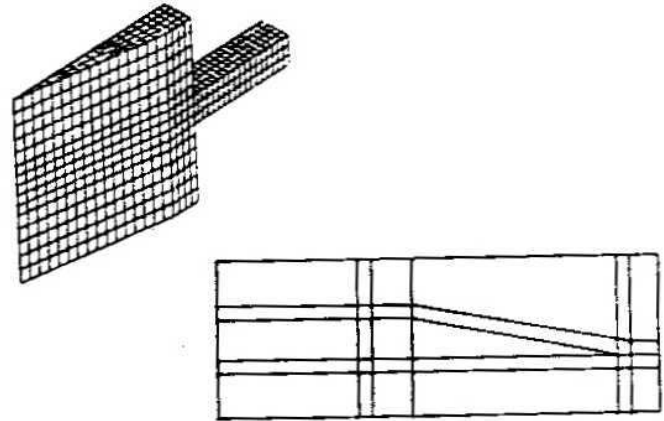
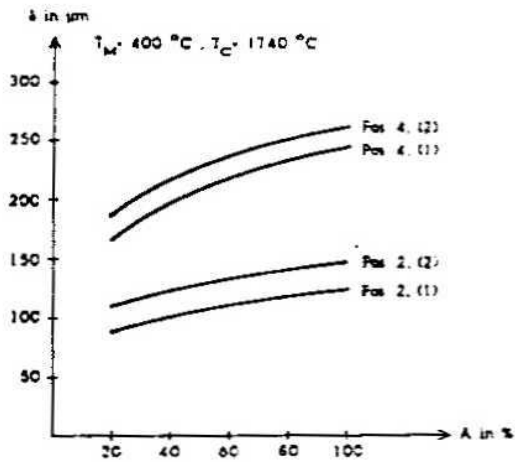


Fig. 7 - Layer thickness is also dependent on melt admission conditions in the mould. The figure shows the dependence of layer thickness on the investment mould acceleration moment at top (1) and bottom (2) of the wedge

Fig. 8 - Meshing for FEM simulation

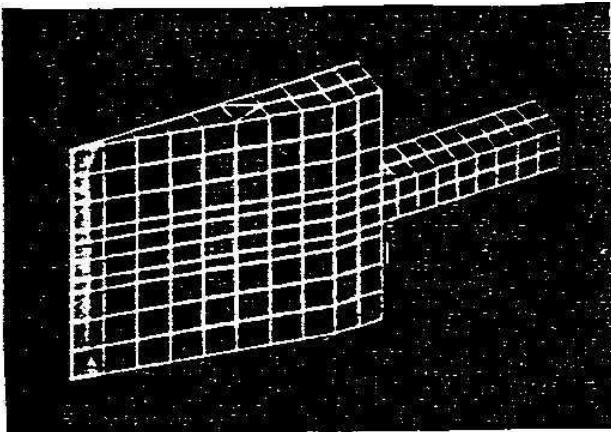


Fig. 9 - Using the CASTS programme package produced at the Institute, temperature distribution for any desired time increment can be calculated

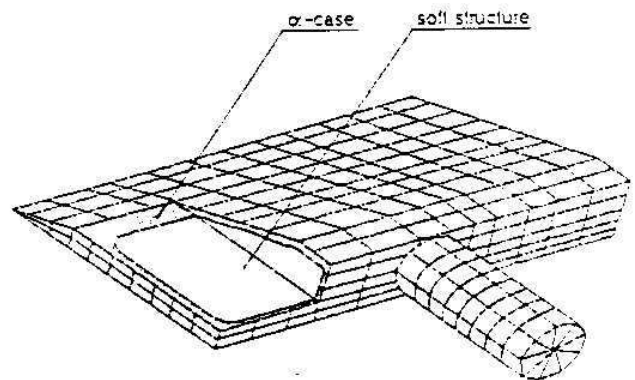


Fig. 10 - The thickness of the alpha-case layer can be visualized for any desired section through the casting

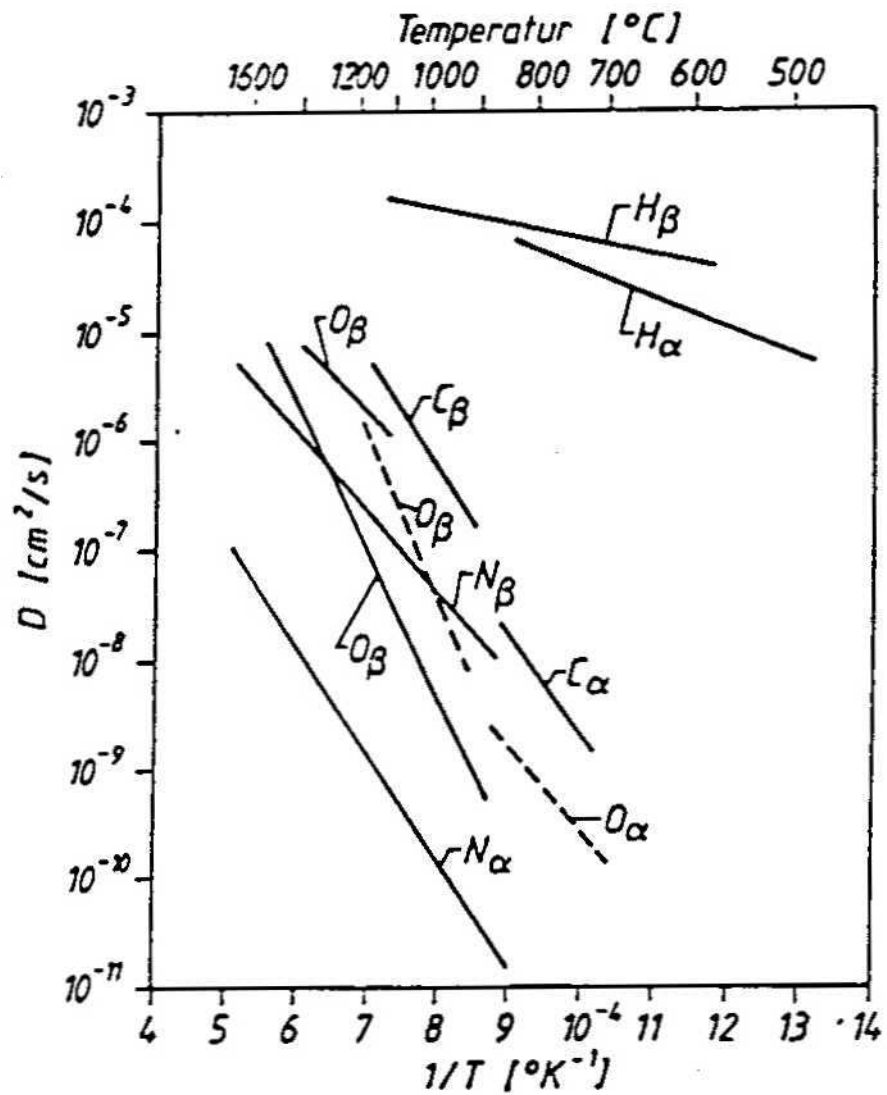


Diagram 1 - Diffusion of hydrogen, oxygen and nitrogen in alpha and beta titanium (9)